RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 48, NUMBER 6 1 AUGUST 1993-II

Numerical study of localization of Dirac fermions on a lattice in two dimensions

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(Received 8 June 1993)

We studied the effects of impurities on Dirac fermions numerically. We used a tight-binding Hamiltonian of fermions with the magnetic flux equal to π per plaquette for the model. A small amount of strong impurities create states near the zero energy and strong localization of these states is observed. Our results support a recent proposal of localization effects in a gapless d-wave superconductor.

There is strong interest in the possibilities of d-wave pairing in oxide superconductors[1–3] and the effect of impurities on this state. In particular, one of us[1] has argued that a small concentration of strong impurities (unitary limit) creates strongly localized states in the gap near zero energy for a two-dimensional d-wave superconductor with short coherence length. The analytic theory is based on the application of the scaling theory of localization and it is useful to check this numerically. Instead of a superconductor problem that involves the introduction of an off-diagonal order parameter, we focus on a different problem that should show the same physics.

The important feature of d-wave superconductivity is that the energy gap closes linearly along a direction parallel to the Fermi surface. Near this zero point, the energy gap can be described approximately with a two-dimensional massless Dirac fermion. Therefore we investigate the effects of disorder on Dirac fermions in two dimensions. This problem is theoretically interesting by itself and has not received much attention up to now. Furthermore, Dirac fermions appear in the transition between different quantum Hall states[4–7] and our problem may be relevant to an impurity-driven transition between quantum Hall plateaus.

To do a numerical simulation, we have to realize the Dirac fermion on a lattice. We used a tight-binding model with a uniform magnetic field on a square lattice. When the magnetic flux through the plaquette, ϕ, is p/q with an even integer $q = 2q'$, there are two energy bands with a linear dispersion and which touch at zero energy.[8,9] The most well-known case is the $\phi = \pi$ case that appears in the flux phase, which is considered as an exotic mean-field state of the two-dimensional Hubbard model.[10] This π-flux model has two Dirac fermions and in general, the $\phi = p/2q'$ state has q' Dirac fermions near zero energy. We focus on the π-flux case because time-reversal symmetry is preserved in this case. Indeed, the effect of disorder on the π-flux model has been addressed by Fisher and Fradkin, who showed that it belongs to the universality class of $O(2n, 2n)/O(2n) \times O(2n)$ class σ model.[11] When combined with the observation that the dimensionless conductance of a related model is of order unity,[1] we are led naturally to the conclusion that the states near zero energy become localized.

Our Hamiltonian for the tight-binding model with uniform magnetic field with impurities is given by

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger e^{i\theta_{i,j}} c_j + \text{H.c.} + \sum_{j_r=1}^{N_{\text{imp}}} V_{j_r}^{\text{imp}} c_{j_r}^\dagger c_{j_r}, \quad (1)$$

where $c_j^\dagger$ is a creation operator of the lattice fermion at site j and the last term is a random potential V_{j_r} at random sites j_r. A distribution of the random potential is assumed to be uniform between $[-V/2, V/2]$. The phase factor $e^{i\theta_{i,j}}$ is chosen such as $\sum_{\text{plaquette}} \theta_{i,j} = \pi$ to produce the linear dispersion near the zero energy. We used the Landau gauge $\theta_{j,j+\hat{y}} = m\pi$ and $\theta_{j,j+\hat{x}} = 0$ to represent π flux where $j = (m, n)$. When there are no impurities, the Hamiltonian is diagonalized in the momentum representation and the energy bands are given by

$$E(\mathbf{k}) = \pm 2t\sqrt{\cos^2 k_x + \cos^2 k_y} \quad (2)$$

$$\approx \pm 2t\sqrt{(k_x - k_x^i)^2 + (k_y - k_y^i)^2}$$

$$(\mathbf{k} \approx \mathbf{k}^i, \quad i = 1, 2), \quad (3)$$

where $(k_x^1, k_y^1) = (\pi/2, \pi/2)$ and $(k_x^2, k_y^2) = (\pi/2, -\pi/2)$. This model has doubled Dirac fermions located at these two points. We note that the Dirac fermion dispersion is isotropic near $\mathbf{k}^i$. In the d-wave superconductivity problem, this corresponds to a very short coherence length of order of the lattice constant. According to the analysis of Ref. 1, this is the most favorable case for localization. This model without randomness is well studied. In Fig. 1, we plot the energy dispersion of the model. One can see clearly the linear dispersion for the Dirac fermions. We used a Brillouin zone of the original model but the magnetic Brillouin zone is half of this. Therefore the number of Dirac fermions is two. There are several subtleties for the Dirac fermions on the lattice. The Hall conductance of the system is a topological quantity and it is characterized by the response to the boundary condition.[12] A nonzero Hall conductance means an existence of an extended state. When the Fermi energy of the system lies at the zero energy of the π-flux case, the Hall conductance of the system is ill defined. An infinitesimal next-nearest-neighbor hopping t' opens a gap

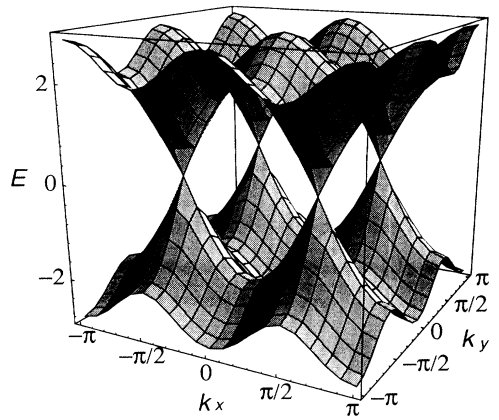

FIG. 1. Energy dispersion of the π-flux model. The Brillouin zone here is that without π flux, the magnetic Brillouin zone is half of this. Thus the number of Dirac fermions is two.

and the Hall conductance is given by $-(t't/|t't|)$.[13,6] It suggests that the Dirac fermion appears when (integer) Hall conductance changes from one integer to the other integer discontinuously.[4–6] Due to these subtleties of this Dirac fermion, the effect of the disorder is a nontrivial problem by itself.

In the following, we show the results of numerical simulation for finite systems. We considered the effects of the randomness in this π-flux model by comparing a case with a usual randomness without a magnetic field. The unit of the energy is set to $t = 1$. In this paper, we mainly study cases with a strong scattering potential, but the impurities are assumed to be dilute, that is, $V >> t$ and $N_{\rm imp}/L^2 << 1$, where L is a linear dimension of the system. This dilute impurity may be comparable to the realistic oxide materials. We remark here that this model preserves the time-reversal symmetry due to the special feature of the π flux.

First let us discuss the density of states for the model. When there is no randomness, there are two energy bands with the Van Hove singularities and the density of states of these two energy bands vanishes linearly at the zero energy. In Fig. 2, we showed density of states for a 36×36 system with $N_{\rm imp} = 20$ and $V = 100t$ for one impurity realization. The density of the impurities is $\approx 1.5\%$ and it is considered as a dilute impurity case. An average over several samples is also performed but the appearance of the states in the gap region is more clearly observed in Fig. 2. For a reference, we plotted the density of states for the system without the random potential (dotted line). In the calculation, we included a small imaginary part $\delta = 0.03t$ to give a finite width to delta functions. Due to the small system size, the spectrum is discrete. However, we can see that the global structure of the density of states remains unchanged. Inclusion of the randomness causes the broadening of the spectrum which is observed in the region $|E| \gtrsim 0.5t$. On the other hand, near the zero energy, some states appear with broadening of the zero energy state ($|E| \lesssim 0.3t$). It suggests that the small amount of the strong disorder creates states near the zero energy which is consistent with the analytic results.[1]

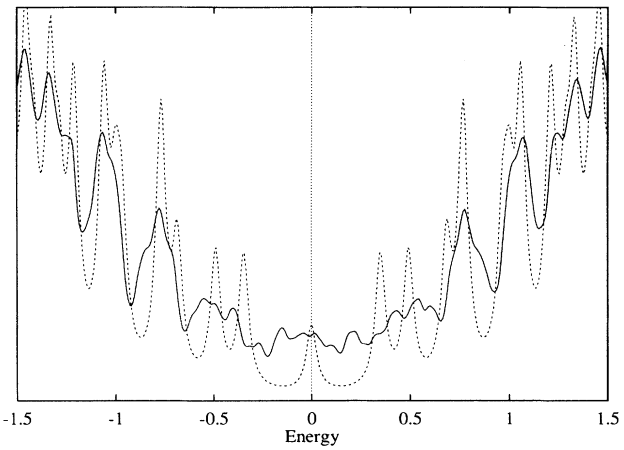

FIG. 2. Density of states for the 36×36 system with π flux (with small imaginary part $\delta = 0.03t$): solid line, $N_{\rm imp} = 20 \approx 1.5\%$ and $V = 100t$; dotted line, the same parameters without the random potential.

Next we study the nature of the eigenstates to see if they are localized. A useful test[14] for the localization is the study of the sensitivity to changes in the boundary condition, $\kappa_j = \partial^2 E_j/\partial\chi^2$ where E_j is the jth eigenvalue with a twisted boundary condition $\Psi(x + L, y) = e^{i\chi}\Psi(x, y)$. For y direction, the periodic boundary condition is used. The results for three different impurity realizations are shown in Fig. 3(a) for the π-flux case in the 36×36 system with $N_{\rm imp} = 20$ and $V = 100t$. For comparison, similar results for the standard Anderson model (i.e., without the π flux) are shown in Fig. 3(b). It is clear that the additional states introduced into the gap in the π-flux case become very insensitive to the change in boundary conditions.

We also calculated the dimensionless conductance, $g(E)$, to study the localization of the system. We used the Thouless formula for $g(E)$ (Ref. 14)

$$g(E) = \frac{1}{\Delta(E)} \left\langle \left(\frac{\partial^2 E}{\partial \chi^2} \right)^2 \right\rangle^{1/2} \Bigg|_{\chi=0}, \tag{4}$$

where $\Delta(E)$ is a local mean level spacing near E and $\langle\ \rangle$ means an average over a small energy range. We note that since $\Delta(E)$ is large in the π-flux case, the dimensionless conductance exhibits the localization effects even more strongly than $\partial^2 E/\partial\chi^2$ itself. In Fig. 4(a), we plot a dimensionless conductance for the π-flux case for the 36×36 system with $N_{\rm imp} = 20$ and $V = 100t$ for three different impurity realizations. In Fig. 4(b), we plot a similar result without magnetic flux. The average is taken over seven local energy eigenvalues. First of all, the dimensionless conductance of the system without a magnetic field is very large and of the order of the system size. It suggests that the impurities are dilute and the mean free path is large. For high energy states of the π-flux case $|E| \gtrsim 0.5t$, fluctuations are large and the values are also of the order of the system size [Fig. 4(b)]. On the other hand, near the zero energy where the dispersion is linear in a pure system, it clearly shows that conductance of the system is strongly suppressed. This

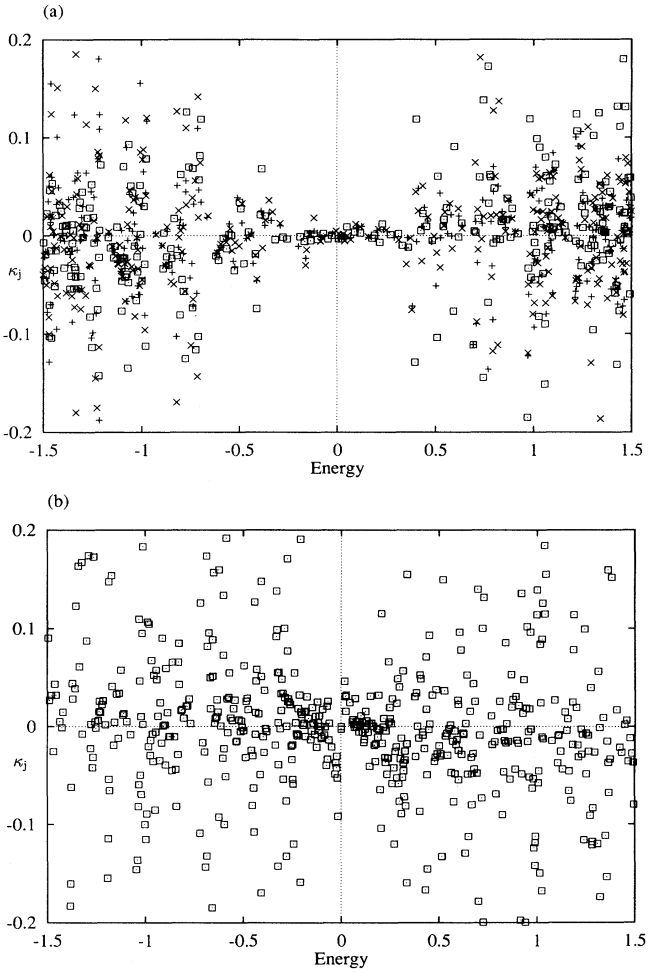

FIG. 3. The sensitivity to changes in boundary conditions, κ_j, for the jth eigenstates of the 36×36 system with $N_{\rm imp} = 20 \approx 1.5\%$ and $V = 100t$. (a) With π flux (different symbols are for different impurity realizations), (b) without flux. The degeneracy at the zero energy in the tight-binding model is not completely lifted by the dilute impurities. We omitted these states from the calculations.

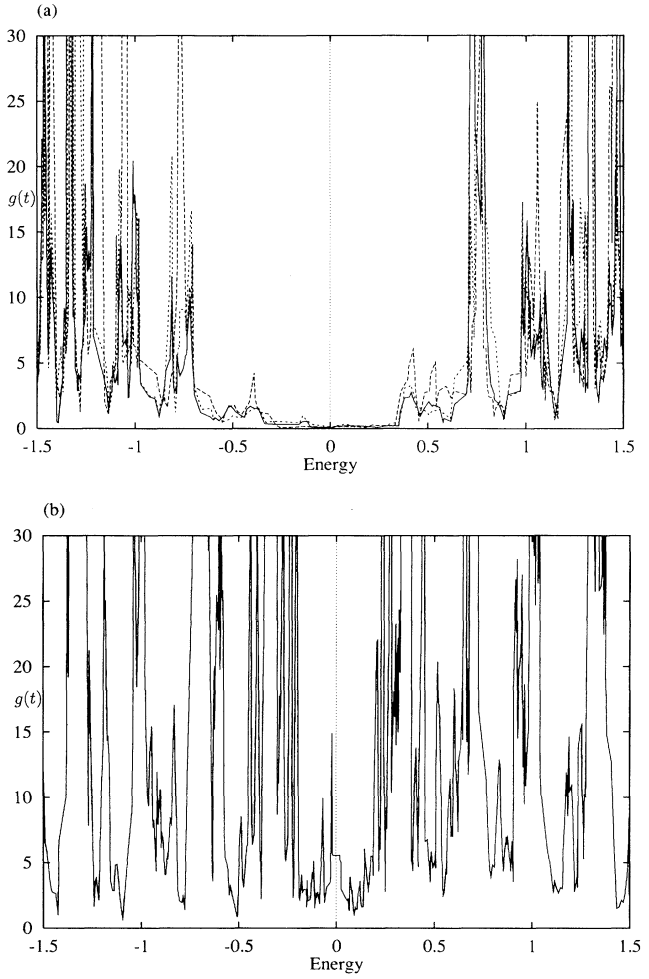

FIG. 4. The dimensionless conductance $g(E)$ for the 36×36 system with $N_{\rm imp} = 20 \approx 1.5\%$ and $V = 100t$. (a) With π flux (different lines are for different impurity realizations), (b) without flux.

is the striking feature of the π-flux case. The conductance is very small $g \ll e^2/h$ in this region. It suggests that the states which appeared near the zero energy are strongly localized even in the dilute impurity case. This result is also consistent with the analytic result.[1] We have also studied an alternate model of disorder when a disorder potential V_i is introduced on every site where V_i is randomly distributed between $\pm V$. In this case, we find that a substantial ratio of V/t is necessary before enough states are introduced near energy zero. Furthermore, the localization of these states is apparent only for $V/t \approx 3$ or 4, when the eigenstate for the standard model (i.e., without the π flux) also begins to show localization for the finite-size system. Thus the introduction of a dense distribution of weak disorder does not have nearly as dramatic an effect on the Dirac spectrum as the introduction of a dilute concentration of strong scatterers. This is also in agreement with the analytic analysis,[1] which shows that the mean free path is very long in the case of Born scattering so that localization effects will not be observed in small lattices.

In summary, we have investigated the effects of impurities for two-dimensional Dirac fermion. We used a π-flux model of tight-binding fermions on a square lattice to realize the Dirac fermions. We have treated systems with dilute but strong scattering potential impurities where the mean free path is large in the absence of the π flux compared to the lattice constant, and the system is a good metal. We observed that upon the introduction of the π flux some states are created near the gap region and the dimensionless conductance of these states is very small ($g \ll e^2/h$), which suggests such states are strongly localized. To obtain quantitative results, we have to do more extensive calculations and an average over many samples may be necessary. However, our numerical results qualitatively support the analytical results.[1]

This work was supported by NSF through the Material Research Laboratory under Grant No. DMR-9022933. Y.H. is grateful to X. G. Wen for many helpful discussions.

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[1] P. A. Lee (unpublished).
[2] N. Bulut and D. J. Scalapino, Phys. Rev. Lett. **68**, 706 (1992); J. A. Martindale et al., *ibid.* **68**, 702 (1992).
[3] For example: T. R. Thurston *et al.*, Phys. Rev. B **46**, 9128 (1992); Z. -X. Shen *et al.*, Phys. Rev. Lett. **70**, 1553 (1993); S. E. Basrrett *et al.*, *ibid.* **66**, 108 (1991); M. Takigawa, J. Smith, and W. Hults, Phys. Rev. B **44**, 7764 (1991)
[4] X. G. Wen and Y. S. Wu, Phys. Rev. Lett. **70**, 1501 (1993).
[5] W. Chen, M. P. A. Fisher, and Y. S. Wu (unpublished).
[6] The appearance of the Dirac fermions at a transition between different integer quantum Hall states on a lattice is discussed in Y. Hatsugai and M. Kohmoto, Phys. Rev. B **42**, 8282 (1990).
[7] Matthew P. A. Fisher (private communications).
[8] M. Kohmoto, Phys. Rev. B **39**, 11943 (1989).
[9] X. G. Wen and A. Zee, Nucl. Phys. **B316**, 641 (1989).
[10] I. Affleck and J. Marston, Phys. Rev. B **37**, 3774 (1988); G. Kotliar, *ibid.* **37**, 3663 (1988).
[11] M. P. A. Fisher and E. Fradkin, Nucl. Phys. **B251** [FS13], 457 (1985); E. Fradkin, Phys. Rev. B **33**, 3257 (1986); **33**, 3263 (1986).
[12] D. J. Thouless, M. Kohmoto, P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).
[13] X. G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B **39**, 11413 (1989).
[14] D. J. Thouless, Phys. Rep. **13C**, 93 (1974).